SOME APPLICATIONS OF MODELS TO AIR TOXICS IMPACT ASSESSMENTS

by

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Application of Air Models to Natural Resource Injury

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PREFACE

Air toxics are of increasing concern to Federal and State air pollution control agencies. As with criteria air pollutants (e.g., SO_2, TSP, CO, O_3, NO_x, Pb), ambient impact assessments for air toxics frequently must be based on dispersion models. However, air toxics present unique problems in mathematically simulating the emissions characteristics and the atmospheric transport, transformation, and removal of these pollutants. While models are available for many toxic pollutants and emissions situations, frequently they are not widely known or tested.

The purpose of this report is to identify models that are available for toxics impact assessments and factors that should be considered in selecting models for specific applications. There is no claim as to the merits of individual models or that the list of models is comprehensive. This report only provides information that may be considered useful to air pollution control programs concerned with air toxics and should not be construed as providing regulatory guidance.

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1.0 INTRODUCTION

The assessment of air toxics impacts requires analyses of a wide range of pollutant release types and atmospheric phenomena over varying time and distance scales. Simulation of all aspects of such releases is not possible using a single model or modeling approach. Often, the issues addressed in modeling assessments are at the limits of our current knowledge of atmospheric dispersion phenomena as related to source release characteristics.

Models used for air toxics impact assessments consist of components for simulation of source emissions, transport and dispersion, chemical transformations, and deposition. Table 1-1 lists a sample of components that might be considered in simulating the emission of material and initial dispersion of pollutants. Requirements for simulation of transport, dispersion, and deposition are not included in this table. These may require significantly more detail than is commonly considered. This suggests the need for caution in applying the techniques and the need for expert assistance in the more complicated assessments.

This report consists of five technical sections. Section 2.0 provides a summary description of air toxics releases and characteristics of models. Section 3.0 identifies a method for selection of appropriate modeling techniques by outlining the components of assessment methods for characterizing different types of releases. Section 4.0 provides a catalog of available modeling techniques. Section 5.0 presents a summary of previous performance evaluations of models and a statement on potential modeling uncertainties. Section 6.0 provides a summary and general comments on modeling techniques. An extensive list of references provides additional information on models.

TABLE 1-1

POTENTIAL COMPONENTS OF SOURCE AND INITIAL DISPERSION MODELS

Structure Effects

Flow obstructions
Multiple stack plume rise modifications
Stack tip downwash
Wake cavities and effects

Plume Rise

Buoyant
Momentum jet
Moist
Directional
Flares
Time dependent

Evaporation/Vaporization

Pool spreading
Flashing
Aerosol formation (two phase)
Chemical Transformations
Vapor overflow
Pool vaporization (heat/mass transfer)

Initial Dispersion

Cold gases
Heavy molecular weight gases
Transitional buoyancy gases
Buoyancy induced initial mixing
Gravity spreading (slumping)
Plume liftoff
Particle settling

Uncontrolled Releases (fires)

Buoyant plume rise
Chemical formation

2.0 AIR TOXICS RELEASES AND MODELS

This section summarizes types of impacts associated with air toxics releases. The second subsection discusses the role of models in impact assessments. The third subsection discusses the types of models available.

2.1 Atmospheric Impacts

Air toxics releases can have either prolonged (chronic) or acute impacts on public health and welfare. A prolonged impact is one that does not have an immediate effect on health or welfare, but is the result of accumulated exposure. These impacts are generally related to continuous chemical releases over long periods which cause a persistent low level concentration. Such a long-term impact might result from a situation such as the annual accumulation of a chemical which originates as a slowly evolving volatile emission from a material storage area or material carried in windblown soil particles. An acute impact is one related to short-term, high concentrations of a pollutant resulting in an immediate effect on health or welfare. These short-term impacts are the result of a single event or chemical release causing a one-time concentration. This type of impact might include a plant upset in which an air toxic is released over a period of minutes.

Spatial scales of interest vary by chemical. In general, for long-term impacts, concentration levels may be lower and source receptor distances longer. For short-term impacts, high concentrations are typically of greatest interest and as a result the source/receptor separation distance is generally small. Also, different time scales in combination with the need to simulate source emissions, transport and dispersion, and potential chemical transformations and deposition, require a number of different modeling techniques. These techniques are summarized in Section 2.3.

2.2 The Role of Models in Air Toxics Impact Assessments

The role of models in impact assessments in most cases is to contribute to the general body of knowledge on ambient concentrations. Model selection for assessments is dependent on processes being simulated and data availability. The following sections discuss results generated by different types of modeling requirements to simulate physical and chemical processes of interest. Data availability is crucial in determining the uncertainty in information. Poor data will not support good models and, as a result, a weak data base may require that a simplified model be used. From simplified models, less precise conclusions are usually drawn for the impact assessment.

2.3 Characteristics of Models

Complete dispersion models are those which simulate all important aspects of contaminant behavior from the source to the receptor. Such models are generally constructed from collections of component modules or submodels. Submodels simulate individual processes affecting the fate of pollutants but do not provide the entire answer to the source/receptor relationship.

The basic model components for short- and long-term impacts can be characterized as source and emissions, transport and dispersion, and chemical transformation and deposition modules.

2.3.1 Source Types and Emissions Modules

Sources are typically distinguished as being point, line, area or volume sources, with emissions specified in units of rate, rate per line length, or rate per area. Assessment of air toxics impacts often requires complex descriptions of sources through emission modules. Some of the characteristics of sources identified in this study are as follows:

Point Sources - Point sources of air toxics are frequently characterized as being continuous (steady state) or time dependent. Traditional air quality models use continuous point source parameters in determining steady state solutions to diffusion equations. Source inputs to the models include a constant emission rate and source release height, and parameters for simulating plume rise (i.e. exhaust flow rate, exit temperature and stack diameter). Phenomena simulated are typically limited to stack tip downwash for low velocity releases, buoyancy induced dispersion, and momentum plume rise equations for high velocity, neutral buoyancy plume rise. Models in the Guideline on Air Quality Models (U.S. EPA, 1978) are adequate to simulate these releases.

Air toxics impact studies could potentially require simulation of time dependent emissions, emissions and plume rise from fires and flares, and directional releases. Time dependent releases are often from pressure drops associated with leaks and venting from pressure vessels and pipelines. Emissions modules for establishing the release rates for pipelines are available (e.g. Hanna and Munger, 1983; Blewitt, 1985). Emission rates from fires are not generally described in the literature due to the difficulty in identifying the general chemical composition of combustion products. Plume rise for fires and flares can be determined by buoyant and jet plume rise equations. The simulation of directional plume rise is most important for high momentum jets and is sometimes simulated by estimating the vertical momentum component.

Line Sources - Line sources are most commonly used to describe mobile source effects. Some of the applications for which line source descriptions are applicable for air toxics are the spraying of agricultural pesticides and herbicides and vapor releases over berms.

Area Sources - Typical area source applications for air quality modeling include simulations of large areas of poorly defined sources and areas of fugitive dust generation due to industrial and agricultural activity or wind blown dust. Area sources in air toxics modeling may be of the following types:

-- emissions for small or poorly defined sources located in urban areas or industrial complexes (e.g. fugitive emissions).

-- evaporation from liquid spills in confined areas (e.g. dikes).

-- vaporization from spills of liquefied gases in confined areas.

-- heavy gas leaks in confined areas.

-- evaporation from liquids and liquified gases spreading on water.

-- emissions from waste disposal operations, (e.g. landfills, land treatment, surface impoundments, waste water treatment units).

Modeling volatile liquids and liquefied gases in unconfined spills on water provide the most complicated cases as they require simulation of both spreading and evaporation in a time dependent emissions module. These modules are described in more detail in Section 4.2.1.

Volume Sources - In air quality modeling, volume sources are seldom considered in explicit solutions to diffusion equations. Sources are sometimes defined to represent the volume generated in the wake zones of flow obstructions such as buildings. Downwash models are important in air toxics applications, but more common is the requirement to define an initial cloud resulting from the rapid vaporization of liquefied gases. In refrigerated liquefied gas spills on land, rapid vaporization results from soil surface heating; vaporization models show a decrease in vaporization rate with time. For pressurized liquefied gases, a rapid vaporization (flashing) due to adiabatic decompression occurs. For example, in a liquid chlorine spill from a typical pressurized storage vessel, 20 percent of the gas may be flashed. The turbulence of this gas entrains air to build an almost instantaneous cloud

of perhaps ten times the volume of the gas. The situation is more complex if a pressurized storage vessel is damaged below the liquid level. In this instance, rapid boiling causes the generation of a gas and aerosol cloud which could include the major portion of liquid in the tank.

2.3.2 Dispersion Models

Air quality dispersion models for assessment purposes are typically of the continuous emission source, Gaussian dispersion type that handle buoyant or neutrally buoyant gases and aerosols. For air toxics applications, two modifications to this approach are sometimes needed. First, simulations for acute impacts may require instantaneous or puff solutions to diffusion equations and second, negatively buoyant plumes may require simulation using a gravity spreading or slumping model.

Continuous emission source dispersion models, as represented by the EPA Guideline on Air Quality Models, incorporate model components including:

- point, line and area equations
- momentum and buoyant plume rise
- building and stack tip downwash
- variations in averaging periods
- multisource and multiple pollutant capabilities
- limited terrain and deposition capabilities

Neutrally buoyant instantaneous sources are simulated with an alternative and generally accepted puff solution to the diffusion equations. Models are available representing time dependent sources by sequences of steady state puffs or plume elements for simulating dispersion in temporally and spatially changing wind fields. Both continuous and instantaneous models are used in conjunction with slumping models to simulate heavy gas dispersion.

2.3.3 Chemical Transformation and Deposition Models

Chemical transformations and deposition can be very important in air toxics impact modeling when the initial generation of toxic byproducts and the materials losses en route between a source and receptor are being simulated. The initial chemical reactions are typically determined on a chemical specific basis as part of an emission specification. For example, several tetrachloride compounds react with water vapor in air to form HCl droplets. An initial assumption for modeling may be that the reactions go to completion prior to dispersion. Modeling of chemical transformations downwind might also take the form of a linear transformation rate which, in simplified Gaussian models, would involve an exponential loss (or gain) term.

Deposition losses are difficult to simulate due to our limited current understanding of this phenomena. Estimates of wet deposition require a further understanding of whether the scavenging takes place in the subcloud layer or by incorporation of the contaminant in the cloud system. Proper specification of precipitation rate is very important.

Dry deposition in simplified models is often represented by an exponential decrease in concentration at a rate determined by a gravitational settling velocity (large particles) or a deposition velocity (gases and fine aerosols). These parameters although called velocities are simply the ratios of mass flux of contaminant to the local concentration and are determined empirically. The parameters are site and pollutant specific and little information is available for air toxics applications.

3.0 APPLICATIONS OF MODELS TO AIR TOXICS IMPACT ASSESSMENTS

The sub-sections which follow discuss the use of dispersion models in air toxics impact assessments. Section 3.1 discusses sources of input data. Section 3.2 describes the basis for model selection.

3.1 Alternative Data Sources

Data for dispersion modeling must be representative of the conditions which govern emissions and transport. Dispersion simulations are subject to uncertainties (section 5.1) even when the appropriate data are used. Poor selection of data or data errors increase these uncertainties. As a result, data selection can be as important as model selection.

Data typically required for air toxics modeling are listed in Table 3-1. On-site meteorological data are preferred for modeling analyses. Alternative data sources follow:

Source data:

- review of process data for similar incidents
- determination of chemical characteristics from general references
- examination of reports of the behavior of similar chemicals
- evaluation of processes: mass balances

Meteorological data:

- identification of local representative observation sites
- data collection from the National Climatic Data Center
- review of historical data bases for feasible worst case meteorological conditions

3.2 Model Selection

The description of model characteristics provided in Section 2.0 suggests the complexity which accompanies an impact assessment for air toxics emissions. This section provides techniques for selection of models. Models considered here are of an intermediate complexity in that they provide quantitative results but at the same time are less sophisticated than current

TABLE 3-1

INFORMATION REQUIREMENTS FOR
AIR TOXICS IMPACT ASSESSMENTS

Release

- source type (stack, flare, uncontrolled spill on water, etc.)
- chemical characteristics
- release characteristics
- release height
- release rates
- visible cloud dimensions
- operational characteristics/description of the source
- duration

Meteorology

- wind speed
- wind direction
- stability parameters (wind variation, lapse rate, etc)
- day/night
- mixing height
- temperature
- cloud cover
- date
- precipitation

Site Characteristics

- obstacles to the flow at the release site
- spill surface (land/water)
- characteristics of dispersion route (terrain, snow surface, roughness, etc.)

General Description

- time sequence of release events

research grade models. This level of model complexity was selected to provide a category of techniques useful to a large number of users. Research grade models are recommended when specific source attribution estimates are required in combination with a thorough understanding of processes involved. Use of those models is beyond the intent or scope of this report.

The basis for model selection in this guideline is a decision tree. The decision tree attempts to identify model components required to simulate a particular effect and those components that should be included in complete dispersion models. The decision tree considers simulation of various materials released through different mechanisms (e.g., liquefied gases released on land in confined areas versus a pressurized liquefied gas tank failure). Since many of the physical principles involved in dispersion are shared among release types, the same dispersion models are selected when conditions allow. The decision tree directs the user to subsections of Section 4.0 where complete models or modules are described.

Table 3-2 presents the decision tree used in model selection. Instructions are provided which carry the user through the model selection scheme by considering relevant questions on source and release type, data evaluation and selection, selection of a dispersion model or submodule, and selection of parameters to run the model.

The decision tree in Table 3-2 is used by following the sequence of instructions listed. The tree begins with a decision on whether the impact is associated with long- or short-term releases. The selection establishes a pathway of subsequent decisions and instructions. Instructions through the tree are of three types. The first type is a directional instruction to proceed to another numbered instruction and has the form of a statement "go to (number)". The second form of instruction is an implicit continuation which simply means that if there is no directional instruction, proceed to the next

numbered instruction. The third type of instruction directs the user to specific subsections of Section 4.0 where some model or module is described. After identifying the information in Section 4.0, the user returns to the instruction number to continue the path.

TABLE 3-2

DECISION TREE TO SELECT MODELS
FOR AIR TOXICS IMPACT ASSESSMENTS

DETERMINATION OF RELEASE TYPE

Characterize the impact as either short- or long-term.

1. Short-term - go to 9

2. Long-term - go to 3

LONG-TERM MODELING APPROACHES

3. It is assumed that impacts associated with long-term exposures involve sources with normal releases, persistent fugitive releases, or fugitive releases from either evaporation of volatile material or generation of particles as wind blown dust. Select emission factors based on the following categories:

   3a. Resuspension (wind erosion) generation of particles (Section 4.2.1).
   3b. Evaporation of volatile materials (Section 4.2.1).
   3c. Specified releases of materials from controlled sources or process fugitives. Use measurements of emissions or process estimates.

4. Evaluate available data from the period of emissions. Dispersion models typically require information on wind speed, wind direction and atmospheric stability representative of the source. In addition, data on atmospheric mixing height are very important if the source/receptor separation distance is in excess of a few kilometers. For long-term impacts, data can be supplied to models as sequences of short-term (hourly) data or as joint frequency distributions of wind direction and speed and stability. Lack of on-site data requires an analysis of off-site data resources for representativeness. Feasibility studies determining order of magnitude estimates are possible with judiciously selected or worst case wind data.

5. Select model. EPA has recommended models to simulate dispersion of neutral buoyancy gases in the atmosphere. These models simulate dispersion from point, area and line sources with options to include multiple receptors and sources, varying averaging periods and emissions.

   Options in the models include building wake effects, momentum and buoyant plume rise equations, terrain effects and deposition. The models are typically steady-state Gaussian models using straight line trajectories which limits their range of applicability. Variable trajectory models may be needed for assessments over large source/receptor separation distances or, in areas of locally varying wind fields (e.g. areas influenced by terrain obstacles or local circulations; Section 4.1.2).

TABLE 3-2
(Continued)

DECISION TREE TO SELECT MODELS
FOR AIR TOXICS IMPACT ASSESSMENTS

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5. (Cont.)
   Model selection from the UNAMAP series of models involves an assessment of available information in relation to model inputs. Major differences in models are in the categories of:

   - terrain inputs
   - single versus multiple sources
   - source types
   - frequency distribution versus sequential inputs for meteorological data.

6. Select model input parameters and review model assumptions. Model documentation should be reviewed to determine if all required variables are available and that model assumptions realistically describe the nature of the air toxics impact.

7. Modify models if necessary. Modifications to the model may include:

   7a. Chemical transformations (Section 4.2.2).
   7b. Alternative deposition techniques (Section 4.2.3).
   7c. Alternative plume rise equations (e.g., flares: Section 4.2.4).

8. Perform model simulations.

STOP

TABLE 3-2
(Continued)

DECISION TREE TO SELECT MODELS
FOR AIR TOXICS IMPACT ASSESSMENTS

SHORT-TERM MODELING APPROACHES

9. Determine the probable form of the released material:

   9a. Gas, particles and/or aerosol - go to 10
   9b. Liquid* - go to 14
   9c. Liquefied gases - go to 20
   9d. Dense gas - go to 23

10. Determine if the released material should be simulated as a continuous, or an instantaneous, source. For gas releases, unlike liquids, the distinction between instantaneous and continuous releases is often clear. Various definitions are available to distinguish between the two classes but a simple rule of thumb might be to consider a release instantaneous if the release time is much less than the travel time between the source and the receptor.

    10a. If releases are continuous - go to 15.
    10b. Go to 11 for instantaneous releases.

11. Instantaneous source models allow simulation of dispersion from point, area and volume sources using steady state solutions to diffusion equations. Area and volume sources are represented by virtual point sources or by spatial integrations of the equations. These expressions simplify the representation of building wake effects, and initial dilution for pressurized releases.

    In situations of complex wind fields and/or large suspected source/receptor distances variable trajectory models are advised if sufficient wind data are available.

    11a. Straight line models - Section 4.1.1
    11b. Variable trajectory models-Section 4.1.2

12. Modify the models. Assumptions in the selected models should be evaluated for the specific application. Modifications may be required to simulate factors such as deposition.

13. Perform an analysis. Instantaneous source models typically available provide semi-empirical results in the form of mean concentrations. In realistic concentration fields, peak concentrations can exceed this mean instantaneous value by a large factor (see Section 4.2.5).

STOP

*Liquids are defined as fluids having boiling points above ambient temperatures at ambient pressures for this application.

TABLE 3-2
(Continued)

DECISION TREE TO SELECT MODELS
FOR AIR TOXICS IMPACT ASSESSMENTS

RELEASES OF LIQUIDS

14. Simulations of liquid spills are accomplished with standard dispersion models after accounting for the generation of vapors by evaporation.

    14a. Instantaneous unconfined spills on water (Section 4.2.1) - gravity spreading of the liquid continues until halted by evaporation. Go to 11.
    14b. Continuous spills on water (Section 4.2.1) - gravity spreading of the liquid establishes a steady state spill radius controlled by evaporation rate and spill rate. Go to 15.
    14c. Confined spills on land (Section 4.2.1). Go to 15.

15. Evaluate available data for the period of emissions. Dispersion models typically require information on wind speed, wind direction and atmospheric stability representative of the source. In addition, data on atmospheric mixing height are very important if the source/receptor separation distance is in excess of a few kilometers. Lack of on-site data requires an analysis of other off-site data resources for representativeness. Feasibility studies determining order of magnitude estimates are possible with judiciously selected or worst case wind data.

16. Select model. EPA has recommended models to simulate dispersion of neutral buoyancy gases in the atmosphere. These models simulate dispersion from point, area and line sources with options to include multiple receptors and sources, varying averaging periods and emissions. Options in the models include building wake effects, momentum and buoyant plume rise equations, terrain effects and deposition. The models are typically steady-state Gaussian models using straight line trajectories which limits their range of applicability. If impact is being estimated for large source/receptor separation distances or in areas of locally varying winds it may be necessary to consider variable trajectory models (Section 4.1.2).

    Model selection from the UNAMAP series of models requires an assessment of available information in relation to required model inputs. Major differences in models are in the categories of:

    - terrain inputs
    - single versus multiple sources
    - source types

17. Select model input parameters and review model assumptions. Model documentation should be reviewed to determine if all required variables are available and that model assumptions realistically describe the impact.

TABLE 3-2
(Continued)

DECISION TREE TO SELECT MODELS
FOR AIR TOXICS IMPACT ASSESSMENTS

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18. Modify models if necessary. Modifications to the model may include:

    18a. Chemical transformations (Section 4.2.2).
    18b. Alternative deposition techniques (Section 4.2.3).
    18c. Alternative plume rise equations (e.g., flares: Section 4.2.4).

19. Perform model simulations.

STOP

LIQUEFIED GAS SPILLS

20. Liquefied gases represent the most complicated source of air toxics due to the effects of pressurization and/or refrigeration required for storage.

    Simulation of these gases involves models which are currently under development and may not be adequately tested for impact assessments (Section 4.1.2). As an approximation, the first step in analysis is a determination of whether the gas is pressurized or refrigerated. If the gas is both refrigerated and pressurized, the most immediate effects will result from the pressurization and this factor would be simulated either concurrently or before the effects of the refrigeration are considered.
    20a. Pressurized liquefied gas - go to 21
    20b. Refrigerated liquefied gas - go to 22

PRESSURIZED GASES

21. Models for pressurized gases should distinguish the source of the gas spill (see sub-models for pressurized gases in Section 4.2.1).

    21a. Spills above the liquid level of a tank, a flashing module will estimate the fraction of material immediately vaporized due to adiabatic decompression. This gas is often treated as an instantaneous release and is simulated as in Step 11 if the buoyancy is near neutral with respect to air. Heavy gases resulting from partial refrigeration, cooling by decompression or those with high molecular weights should be simulated using Step 23.
    21b. Spills below the liquid level of a storage vessel will be simulated as in step 21a except for a provision to estimate gas droplet formation due to rapid boiling in the vessel. The added mass is often assumed to vaporize rapidly and it is added to the initial plume volume prior to simulation as a neutral gas under Step 11 or a dense gas under Step 23.

TABLE 3-2
(Continued)

DECISION TREE TO SELECT MODELS
FOR AIR TOXICS IMPACT ASSESSMENTS

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22. Simulation of refrigerated liquefied gas vaporization is described in Sections 4.2.1. Dispersion modeling of the gas is in the category of

    22a. Negatively buoyant gas clouds - go to 23, or
    22b. Buoyant or neutrally buoyant source models - go to 11

DENSE GAS DISPERSION

23. Models for dense gas dispersion are described in Section 4.1.2. Typical models simulate initial phases of dispersion by slab models where plume spreading is a result of gravitational forces until plume heating (in the case of a cold gas) and entrainment of environmental air dilute the plume sufficiently that atmospheric turbulence takes over as the dominant force in dispersion.

24. Simulations of dense gas dispersion can follow general procedures outlined for short-term exposures, but models specific to negatively buoyant gas clouds (Section 4.1.2) should be substituted for standard Gaussian dispersion models from the UNAMAP series.

    24a. continuous pool evaporation - go to 15
    24b. Initial or instantaneous vaporization - go to 11

4.0 AVAILABLE MODELING TECHNIQUES

Air toxics impact assessments require a wide variety of modeling techniques. This section is provided to identify some of these techniques and to summarize model components. Section 4.1 describes complete models used previously in assessment studies. The models included were derived primarily for air quality applications, but models for chemical and fuels safety assessments are also included. Section 4.2 reviews the techniques used in simulating some of the complex aspects of air toxics dispersion.

4.1 Complete Models

The decision tree in Table 3-2 attempts to include all aspects of dispersion modeling to assure that releases of differing types are simulated using a complete complement of appropriate techniques. The method of analysis uses complete models designed to simulate a particular type of release. In keeping with this idea, the following two subsections describe complete models currently available for simulations. The first section describes EPA models in the UNAMAP modeling system. The second section describes models which were identified through the literature search. The latter category includes instantaneous and heavy gas dispersion models.

4.1.1 Environmental Protection Agency Models on the UNAMAP System

EPA provides numerous models for air quality simulations through the User's Network for Applied Modeling of Air Pollution (UNAMAP). Currently UNAMAP Version 5 provides FORTRAN programs and model users manuals for over thirty models and data processors supporting the models. UNAMAP models are divided into two classes, guideline and non-guideline. Guideline models have been evaluated by EPA and deemed appropriate for simulations in regulatory applications as reported in the Guideline on Air Quality Models (EPA, 1978).

The Guideline (currently under revision) also provides descriptions and suggestions for a variety of model related topics such as model and data selection, uncertainty of models, regulatory applications of models and details such as simulating chemical transformations, deposition and plume rise. Non-guideline models in the UNAMAP system are typically those undergoing development or evaluation, those with duplicate capabilities or those with features not yet endorsed by EPA for regulatory applications.

Models in UNAMAP are generally Gaussian dispersion models for continuous emissions sources. As a class, they are single or multisource and include plume rise equations. Some of the models include provisions for downwash, terrain considerations, deposition through settling, and trapping by inversion layers. Also identified are models which simulate variable trajectories to show the effects of temporally and spatially varying wind fields. For air toxics assessments, the UNAMAP models are appropriate for simulations of continuous or quasicontinuous releases of materials that behave in the atmosphere as neutrally buoyant tracers. These conditions cover a majority of air toxics releases.

The following are brief descriptions of the guideline and non-guideline models appropriate to air toxics assessments:

Guideline Models:

RAM Gaussian-Plume Multiple Source Air Quality Algorithm - This short-term Gaussian steady-state algorithm estimates concentrations of stable pollutants from urban point and area sources. Hourly meteorological data are used. Hourly concentrations and averages over a number of hours can be estimated. Briggs plume rise is used. Pasquill-Gifford dispersion equations with dispersion parameters developed for urban areas are used. Concentrations from area sources are determined using the method of Hanna, that is, sources directly upwind are considered representative of area source emissions affecting the receptor. Special features include determination of receptor locations downwind of significant sources and determination of locations of uniformly spaced receptors to ensure good area coverage with a minimum number of receptors.

Reference - Turner, D.B, and Novak, J.H., 1978: User's Guide for RAM. Vol. I. Algorithm Description and Use. EPA-600/8-78-016A (NTIS Accession Number PB-294 791), Vol. II. Data Preparation and Listings. EPA-600/8-78-016B (NTIS Accession Number PB-294 792). U.S. Environmental Protection Agency, Research Triangle Park, NC. (November 1978).

CRSTER - This algorithm estimates ground-level concentrations resulting from up to 19 collocated elevated stack emissions for an entire year and prints out the highest and second-highest 1-hr, 3-hr, and 24-hr concentrations as well as as the annual mean concentrations at a set of 180 receptors (5 distances by 36 azimuths). The algorithm is based on a modified form of the steady-state Gaussian plume equation which uses empirical dispersion coefficients and includes adjustments for plume rise and limited mixing. Terrain adjustments are made as long as the surrounding terrain is physically lower than the lowest stack height input. Pollutant concentrations for each averaging time are computed for discrete, non-overlapping time periods (no running averages are computed) using measured hourly values of wind speed and direction, and estimated hourly values of atmospheric stability and mixing height.

References - Monitoring and Data Analysis Division, 1977: User's Manual for Single-Source (CRSTER) Model. U.S. Environmental Protection Agency, Research Triangle Park, NC EPA-450/2-77-013. (NTIS Accession Number PB-271 360).

CDM - The Climatological Dispersion Model determines long-term (Seasonal or Annual) quasi-stable pollutant concentrations at any ground level receptor using average emission rates from point and area sources and a joint frequency distribution of wind direction, wind speed, and stability for the same period.

Reference - Busse, A.D., and Zimmerman, J.R., 1973: User's Guide for the Climatological Dispersion Model. Environmental Monitoring Series, EPA-R4-73-024, (NTIS Accession Number PB-227-346). U.S. Environmental Protection Agency, Research Triangle Park, NC. 131 pp. (December 1973).

CDMQC - This algorithm is the Climatological Dispersion Model (CDM) altered to provide implementation of calibration, of individual point and area source contribution lists, and of averaging time transformations. The basic algorithms to calculate pollutant concentrations used in the CDM have not been modified, and results obtained using CDM may be reproduced using the CDMQC.

Reference - Brubaker, K.L., Brown, P., and Cirillo, R.R., 1977: Addendum to User's Guide for Climatological Dispersion Model. Prepared by Argonne National Laboratory for the U.S. Environmental Protection Agency, Research Triangle Park, NC. EPA-450/3-77-015. (NTIS Access Number PB-274 040). (May 1977).

MPTER - MPTER is a multiple point-source Gaussian model with optional terrain adjustments. MPTER estimates concentration on an hour-by-hour basis for relatively inert pollutants (i.e., SO_2 and TSP). MPTER uses Pasquill-Gifford dispersion parameters and Briggs plume rise methods to calculate the spreading and the rise of plumes. The model is most applicable for source-receptor distances less than 10 kilometers and for locations with level or gently rolling terrain. Terrain adjustments are restricted to receptors whose elevation is no higher than the lowest stack top. In addition to terrain adjustments, options are also available for wind profile exponents, buoyancy induced dispersion, gradual plume rise, stack downwash, and plume half-life.

Reference - Pierce, T.E. and Turner, D.B., 1980: User's Guide for MPTER: A Multiple Point Gaussian Dispersion Algorithm with Optional Terrain Adjustment. EPA-600/8-80-016, (NTIS Accession Number P880-197 361). U.S. Environmental Protection Agency, Research Triangle Park, NC. 239 pp. (April 1980).

BLP - BLP (Buoyant line and point source dispersion model) is a Gaussian plume dispersion model designed to handle unique modeling problems associated with aluminum reduction plants, and other industrial sources where plume rise and downwash effects from stationary line sources are important. POSTBLP and BLPSUM are related postprocessors in this system.

Reference - Schulman, L.L., and Scire, J.S., 1980: Buoyant line and point source (BLP) dispersion model user's guide. Document P-73048. Prepared for the Aluminum Association, Inc. by Environmental Research and Technology, Inc., Concord, MA. (NTIS Accession Number P881-164 642). (July 1980).

- Addendum/Supplemental Information for BLP. 2 pp. (December 1982). (Distributed as part of UNAMAP, Version 5, Documentation.)

ISCST - The industrial source complex short term model is a steady- state Gaussian plume model which can be used to assess pollutant concentrations from a wide variety of sources associated with an industrial source complex. This model can account for settling and dry deposition of particulates, downwash, area, line and volume sources, plume rise as a function of downwind distance, separation of point sources, and limited terrain adjustment. Average concentration or total deposition may be calculated in 1-, 2-, 3-, 4-, 6-, 8-, 12-, and/or 24-hour time periods. An "N"- day average concentration (or total deposition) or an average concentration (or total deposition) over the total number of hours may also be computed.

References - Bowers, J.F., Bjorklund, J.R., and Cheney, C.S., 1979: Industrial Source Complex (ISC) Dispersion Model User's Guide, Volumes 1 and 2. EPA-450/4-79-030, EPA-450/4-79-031. (NTIS Accession Number P880-133 044, P880-133 051), Office of Air Quality Planning and Standards, U.S. Environmental Protection Agency, Research Triangle Park, NC. (December 1979).

- Addendum/Supplemental Information to the Industrial Source Complex Model. 20 pp. (December 1982). (Distributed as part of the UNAMAP, Version 5, Documentation.)

ISCLT - The industrial source complex long term model is a steady-state Gaussian plume model which can be used to assess pollutant concentrations from a wide variety of sources associated with an industrial source complex. This model can account for settling and dry deposition of particulates, downwash, area, line and volume sources, plume rise as a function of downwind distance, separation of point sources, and limited terrain adjustment.

ISCLT is designed to calculate the average seasonal and/or annual ground-level concentration or total deposition from multiple continuous point, volume and/or area sources. Provision is made for special x, y receptor points that may correspond to sampler sites, points of maxima or special points of interest. Sources can be positioned anywhere relative to the grid system.

References - Same as ISCST (above).

CALINE3 can be used to estimate the concentrations of non-reactive pollutants from highway traffic. This steady-state Gaussian model can be applied to determine air pollution concentrations at receptor locations downwind of "at-grade," "fill," "bridge," and "cut section" highways located in relatively uncomplicated terrain. The model is applicable for any wind direction, highway orientation, and receptor location. The model has adjustments for averaging time and surface roughness, and can handle up to 20 links and 20 receptors. It also contains an algorithm for deposition and settling velocity so that particulate concentrations can be predicted.

Reference - Benson, Paul E. "CALINE3 - A Versatile Dispersion Model for Predicting Air Pollutant Levels Near Highways and Arterial Streets." Interim Report, Report Number FHWA/CA/TL-79/23, Federal Highway Administration, 1979.

Non-Guideline Models:

TEM8 - TEM8 (Texas Episodic Model) is short-term, steady-state Gaussian plume model for determining short-term concentrations of non-reactive pollutants.

Reference - Staff of the Texas Air Control Board. User's Guide to the Texas episodic model. Texas Air Control Board, Permits Section, 6330 Highway 290 East, Austin, TX 78723. (NTIS Accession Number P880-227 572).

TCM2 - TCM2 (Texas Climatological Model) is a climatological steady-state Gaussian plume model for determining long-term (seasonal or annual) arithmetic average pollutant concentrations of non-reactive pollutants.

Reference - Staff of the Texas Air Control Board. User's Guide to the Texas Climatological Model (TCM). Texas Air Control Board, Permits Section, 6330 Highway 290 East, Austin, TX 78723. (NTIS Accession Number P881-164 626).

PAL - Point, Area, Line Source Algorithm. This short-term Gaussian steady-state algorithm estimates concentrations of stable pollutants from point, area, and line sources. Computations from area sources include effects of the edge of the source. Line source computations can include effects from a variable emission rate along the source. The algorithm is not intended for application to entire urban areas but for smaller scale analysis of such sources as shopping centers, airports, and single plants. Hourly concentrations are estimated and average concentrations from 1 hour to 24 hours can be obtained.

References - Petersen, W.B., 1978: User's Guide for PAL - A Gaussian-Plume Algorithm for Point, Area, and Line Sources. EPA-600/4-78-013. (NTIS Accession Number PB-281 306). U.S. Environmental Protection Agency, Research Triangle Park, NC. (February 1978).

- Addendum/Supplemental Information for PAL, HIWAY2, and RAM. 5 pp. (December 1980).

PTPLU - PTPLU is a point source Gaussian dispersion screening model for estimating maximum surface concentrations for 1-hour concentrations. PTPLU is based upon Briggs plume rise methods and Pasquill-Gifford dispersion coefficients as outlined in the workbook of atmospheric dispersion estimates. PTPLU is an adaptation and improvement of PTMAX which allows for wind profile exponents and other optional calculations such as buoyancy induced dispersion, stack downwash, and gradual plume rise. PTPLU produces an analysis of concentration as a function of wind speed and stability class for both wind speeds constant with height and wind speeds increasing with height. Use of the extrapolated wind speeds and the options allows the model user a more accurate selection of distances to maximum concentration. PTPLUI is the interactive version of this model.

HIWAY2 - HIWAY2 is a batch and interactive program which computes the hourly concentrations of non-reactive pollutants downwind of roadways. It is applicable for uniform wind conditions and level terrain. Although best suited for at-grade highways, it can also be applied to depressed highways (cut sections). HIWAY2 is intended as an update to the hiway model. HIWAY2I is the interactive version of this model.

References - Petersen, W. B., 1980. User's guide for HIWAY2: A highway air pollution model. EPA-600/8-80-018. (NTIS Accession Number P880-227 556). U.S. Environmental Protection Agency, Research Triangle Park, NC. 70 PP. (May 1980).

- Rao, S.T., and Keenan, M.T., 1980: Suggestions for improvement of the EPA-HIWAY Model. J. Air Pollution Control Assoc., 30, 6, 247-256.

- Addendum/Supplemental Information for PAL, HIWAY2, and RAM. 5 pp. (December 1980).

COMPLEX I - Complex I is a multiple point source code with terrain adjustment. It is a sequential model utilizing hourly meteorological input. It assumes a normal distribution in the vertical and a uniform horizontal distribution across a 22.5 degree sector.

Reference - There is no users guide for Complex I, and EPA has no plans to develop one as of December 1980. (Since Complex I is based upon MPTER, the user guide for MPTER is useful. Also note the differences from MPTER given in comment statements in the first few pages of the Complex I source code).

SHORTZ - SHORTZ is designed to calculate the short-term pollutant concentrations produced at a large number of receptors by emissions from multiple stack, building, and area sources. SHORTZ uses sequential short term (usually hourly) meteorological inputs to calculate concentrations for averaging times ranging from 1 hour to 1 year. The model is applicable in areas of both flat and complex terrain, including areas where terrain elevations exceed stack-top elevations. The program requires random-access mass storage capability. An associated compatible meteorological data processor is METZ.

References - Bjorklund, J.R., and Bowers, J.F., 1982: User's Instructions for the SHORTZ and LONGZ Computer Programs, Volumes I and II. EPA-903/9-82-004A and B. (NTIS Accession Number P883-146 092 and P883-146 100). U.S. Environmental Protection Agency, Middle Atlantic Region III. Philadelphia, PA. (November 1982).

LONGZ - LONGZ is designed to calculate the long-term pollutant concentration produced at a large number of receptors by emissions from multiple stack, building, and area sources. LONGZ uses statistical wind summaries to calculate long-term (seasonal or annual) average concentrations. The model is applicable in areas of both flat and complex terrain, including areas where terrain elevations exceed stack-top elevations. The program requires random-access mass storage capability.

References - Same as SHORTZ (above).

MESOPUFF - MESOPUFF is a variable trajectory regional-scale Gaussian puff model especially designed to simulate the air quality impacts of multiple point sources at long distances. Highly user-oriented, MESOPUFF provides a range of flexible options. It is designed to be driven by user-specified meteorological scenarios, of arbitrary duration, constructed by a suitable meteorological preprocessor, MESOPAC. It outputs spatially-gridded concentration arrays averaged over arbitrary time intervals of one hour or more and is designed to

be coupled to a postprocessor, MESOFILE, to provide additional graphical and statistical analyses. Routines are provided for: plume rise, plume growth, fumigation, linear conversion of SO_2 and SO_4, and dry deposition of SO_2 and SO_4.

References - Bass, A., Benkley, C.W., Scire, J.S., and Morris, C.S., 1979: Development of MESOSCALE Air Quality Simulation Models: Volume 1. Comparative Sensitivity Studies of Puff, Plume, and Grid Models for Long-Distance Dispersion. EPA-600/7-80-058 (NTIS Accession Number P880-227 580) U.S. Environmental Protection Agency, Research Triangle Park, NC. (September 1979).

- Benkley, C.W., and Bass, A., 1979: Development of MESOSCALE Air Quality Simulation Models, Volume 3. User's Guide to MESOPUFF (MESOSCALE PUFF) Model. EPA 600/7-80-058) U.S. Environmental Protection Agency, Research Triangle Park, NC. (September 1979).

- Addendum/Supplemental Information for MESOPUFF. 25 pp. (December 1982). (Distributed as part of UNAMAP, Version 5, Documentation.)

4.1.2 Alternative Models

Dispersion for continuous chemical releases can in general be simulated with the continuous models described in the previous section. Table 3-2 indicated situations in which these models would be inappropriate or at least incomplete for a simulation of air toxics emissions. Table 4-1 summarizes the capabilities of a selection of complete models. The table is organized to identify components which are involved in the models under general categories of source, dispersion, chemistry, and deposition components. In addition, details are available about the availability and characteristics of the computer programs. Symbols for the table are described in the footnote. Complete models identified in the table as having codes which are generally available for assessment are described further following the table.

TABLE 4-1

CHARACTERISTICS OF ALTERNATIVE MODELS

MODEL	ALWAS	Tox-Screen	SLAB	INPUFF	SRD DENZ	IEPA	Fuming Acid	OB/DG	EIDSVIK	DDESB	EPA Puff	Van Ulden	AGA	SPILLS*	TOXCOP	HEGADIS -II	SRI PUFF	Germeles and Drake	DEGADIS	Chlorine Institute
Source																				
Point	X**	X	-	X	-	X	X	X	-	X	X	-	-	X	X	X	X	X	-	X
Area	X	X	X	X	X	-	-	-	X	-	X	X	X	X	-	X	-	X	X	X
Line	X	-	-	-	-	-	-	-	-	-	-	-	X	-	-	-	-	-	-	-
Plume Rise	X	X	-	X	-	-	-	-	-	X	-	-	-	X	-	-	-	-	-	X
Downwash	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Pool Evaporation	-	-	-	-	-	X	X	-	-	X	-	-	X	X	X	-	-	X	-	X
Land	-	-	-	-	X	X	X	-	-	X	-	-	X	X	X	-	-	-	-	X
Water	-	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	X	-	-
Pool Spread	-	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	X	-	-
Flashing	-	-	-	-	X	-	-	-	-	-	-	-	-	X	-	-	-	-	-	X
Liquid	-	-	-	-	-	S	X	-	-	X	-	-	-	X	X	-	-	-	-	-
Liquefied Gas	-	-	X	-	X	S	-	-	-	-	-	-	X	X	-	-	-	X	-	X
Gas/Aerosol	X	X	X	X	-	S	X	X	X	X	X	X	X	X	X	X	X	-	X	X
Dispersion																				
Gravity Spread	-	-	X	-	X	-	-	-	X	-	-	X	-	-	-	X	-	X	X	X
Continuous	X	X	X	X	X	X	X	X	X	X	-	-	X	X	X	X	X	X	X	X
Instantaneous	X	-	-	-	X	-	-	-	X	-	X	X	X	X	-	X	X	X	X	X
Straight Line	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
Variable	-	-																		
Trajectory	-	-	-	X	-	-	-	-	-	-	-	-	-	X	-	-	X	-	-	-
Cloud Heating			X	-	X	-	-	-	X	-	-	-	-	-	-	X	-	X	X	-
Chemistry	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Deposition																				
Wet	X	X	-	-	-	-	-	-	-	X	-	-		-	-	-	-	-	-	-
Dry	X	X	-	-	-	-	-	-	-	X	-	-		-	-	-	-	-	-	-
Model																				
Available Code	X	X	X	X	X	-	NS	-	NS	NS	X	NS	X	X	NS	NS	X	NS	X	-
Available Manual	X	X	-	X	X	X	NS	-	NS	NS	X	NS	X	X	NS	NS	X	NS	X	X
Type	C	C	C	C	C	N	C	N	NS	N	PC,N,C	NS	N	C,PC	NS	NS	PC	NS	C	N

*ICARIS is an AAR version of SPILLS

**Symbols
- X Included; - not included
- C Computer
- N Nomogram/calculator
- NS not specified
- PC minicomputer
- S specified

- U.S. Environmental Protection Agency

Model: ALWAS

General Description:

ALWAS is the air, land, water analysis system designed to simulate the fate of airborne toxic materials on the land and surface water. The major component is the DiDOT, Dispersion/Deposition of Toxics, model which simulates the source of toxic material in terms of emission rates from point and area sources; dispersion, using a continuous Gaussian model; and wet and dry deposition with a submodel. The dispersion model was developed and is used to simulate TSP and any other chemical. An option of the model allows interaction of volatile organics and TSP to simulate surface absorption. Dispersion in the model is simulated using techniques from EPA-approved models.

Dry deposition is simulated using a surface depletion model and wet deposition is simulated using a scavenging ratio technique. Wet deposition calculations are provided only to estimate the flux of material from the surface rather than providing an estimate of plume depletion en route between the source and the receptor. The model simulates concentration and deposition values by use of a sequence of hourly data. Modifications are discussed in the user's manual to simulate instantaneous source releases. Inputs to the model include source and meteorological data and chemical specific parameters for wet and dry deposition.

Reference: Tucker et.al. (1984)

- U.S. Coast Guard

Model: DEGADIS

General Description:

DEGADIS, the Dense Gas Dispersion Model has been developed for inclusion in the Hazard Assessment Computer System (HACS) to simulate dispersion of heavy gas releases. The model is a modified version of the HEGADIS-II model, Colenbrander (1980). DEGADIS uses as input information on vapor generation rate and initial source area to build a vapor cloud by considering entrainment and cloud heating. The cloud has a cylindrical core which is horizontally homogeneous and edges which decrease exponentially in the horizontal. The model includes a gravity spreading or intrusion equation to simulate horizontal spread, vertical and horizontal mixing and equations for energy balances and mass uptake. Equivalent parameters are determined relating the cylinder height and width to equivalent mixing parameters from which concentration estimates can be made. It allows a smooth transition from gravity spreading to passive dispersion as the energy level of the cloud due to buoyancy approaches that of existing atmospheric turbulence.

Reference: Havens and Spicer (1985)

- U.S. Environmental Protection Agency

  Model: TOX-SCREEN

  General Description:

  TOX-SCREEN is a multimedia screening model for long term assessment of transport in the air, soil and surface water. The air pathway model is a simplified Gaussian model for point sources and a simple box model for area sources. The dispersion model results for a given wind direction are assumed to stay constant for the month (i.e. short term concentrations) are simulated by a source depletion model and an exponental decay term. Precipitation scavenging is estimated using a washout ratio and monthly average precipitation.

  Reference: Bicknell et.al. 1985

- U.S. Environmental Protection Agency

  Model: INPUFF

  General Description:

  INPUFF is a single source Gaussian dispersion model which allows dispersion calculations for stationary and moving sources of neutrally buoyant materials in air. INPUFF uses a Gaussian puff dispersion equation in stationary or temporally and spatially varying wind fields provided by the user. The model simulates emissions from a single source at up to 25 receptors for up to 144 meteorological periods of length from minutes to an hour. Puff positions are determined by trajectory calculations. Options in the model allow estimation of plume rise; wind speed at release height; position from a moving source; and, from wind field input, the effects of temporally and spatially varying winds including wind fields representative of pollutant transport in complex terrain.

  As a Gaussian model, INPUFF is limited to steady state simulations of neutral tracer dispersion without chemical transformation and/or depositional losses. Area sources are not directly simulated although use of initial dispersion parameters and virtual point source concepts would allow approximations. The model is not part of an emergency response system.

  Reference: Petersen et al. (1984)

- Safety and Reliability Directorate (SRD) , U.K.

  Model: DENZ

  General Description:

  DENZ is a heavy gas dispersion model which draws on and includes components in other models as options in explaining heavy gas releases. For pool evaporation, DENZ uses the SPILL model of the SRD described in the following subsection. For dispersion, the model uses the formulation of Cox and Roe for gravity spreading of heavy gas with top entrainment and a standard Gaussian dispersion model for passive tracers. The model and manual include provision for source simulations from refrigerated and pressurized vessels and the heavy gas or slumping model includes terms for slumping, cloud heating, air entrainment in the cloud. The dispersion model is a Gaussian puff model.

  DENZ provides estimates of concentrations, areas, and doses as well as cumulative probabilities of exposure (for toxic gases). Input to the model includes control records, source information and parameter constants and meteorological data for the site under study.

  Reference: Fryer and Kaiser (1979)

- Illinois Environmental Protection Agency

  General Description:

  The Illinois EPA uses a set of equations based on a continuous Gaussian equation for ground level point sources for estimating downwind evacuation distances. In addition to the dispersion model, the equations also provide estimates for pool evaporation and specifications for continuous and instantaneous discharges of gas or volatile leaks on land and water. The evaporation rate is determined only by the vapor pressure of the material released.

  The model is very simple in its specification of release amounts and simulation of dispersion. Its use is intended to provide a rough estimate of evacuation corridors.

  Reference: Kelty (1984)

- U.S. Environmental Protection Agency

  Model: Instantaneous Puff

  General Description:

  The EPA puff model is an instantaneous Gaussian point source model for ground level sources. It includes provisions for using instantaneous horizontal dispersion parameters and specified initial dispersion rates which give it the ability to simulate area sources by virtual point source techniques. Methods are included for dose calculations and approximating concentrations for time periods other than those for which the initial calculations were performed.

  The puff model is limited as a Gaussian model to simulations of dispersion for neutral buoyancy releases from instantaneous sources.

  Reference: Petersen (1982)

- American Gas Association

  Model: LNG Spills in Dikes

  General Description:

  The AGA has provided a model for LNG spills on flat and sloped dike floors which considers vaporization, dike filling by liquid and vapor and dispersion. Dispersion calculations are performed using a continuous Gaussian line source model without a parameterization for heavy gas spreading. The vaporization model uses previous studies to estimate the boiling rate in conjunction with a series of equations for liquid releases and the geometry of liquid spreading on flat and sloped floors. Estimates are included for the time required before bermed areas are filled by vapors and overflow causing downwind transport.

  The model includes a mix of assumptions which make it in some ways general and in some ways very specific to LNG. Gravity spreading of vapor is neglected and dispersion is simulated using a Gaussian (neutral buoyancy) model, but the boiling model is specific to LNG.

  Reference: AGA (1978)

- Shell Development Company

  Model: SPILLS

  General Description:

  SPILLS is a widely used model for simulation of liquid spills or gas releases on land and the subsequent dispersion of the gases or vapors. The dispersion model is a Gaussian puff model which uses continuous plume dispersion parameters and has the capability of simulating elevated sources and inversion trapping. Area sources are simulated using a virtual point source formulation with the initial dispersion parameters. Source models are of several types. For routine stack emissions, the model uses Briggs plume rise equations. For liquid spills, the model differentiates among continuous leaks and instantaneous spills of a liquefied gas or a liquid. All spills are assumed to be bounded. For continuous leaks, the spill rate is calculated and used as the emission rate with a pool area calculated to provide an area source. For instantaneous sources of liquefied gases, the flashing of gas is calculated, the area of the pool defined and boiling estimated as a result of conductive soil heating and convective heating from the air to provides a time dependent rate. For liquids, a mass transfer model is used. The model is unsteady in that emissions and meteorological conditions change. Puffs released under different conditions are integrated at the receptors of interest.

  The model was prepared for simulating releases of 36 chemicals but is appropriate to others. It is limited in its ability to simulate peak instantaneous concentrations and does not include provisions for pool growth and gravity spreading.

  References:

  - Fleischer (1980)
  - Kricks et al. (1983)
  - Pan et. al. (1983)

- U.S. Coast Guard

  Model: HACS

  General Description:

  HACS is the Hazard Assessment Computer System which contains 18 models describing chemical spills and dispersion. The system is under revision after reviews of early models indicated that significant errors in the models could exist (Tebaugh, personal communication, 1985). One model under revision is the heavy gas dispersion model for which a new model DEGADIS has been developed.

References:

Colonna et. al. (1984)
Potts (1981)
Harding et. al. (1978)

- SRI, International

Model: SRI PUFF

General Description:

The SRI PUFF model is a microcomputer based dispersion model for simulation of unsteady emissions in temporal and spatially varying wind fields. The model calculates non-divergent wind fields from multiple stations, estimates plume positions, determines the puff release rate to assure a continuous plume simulation, and estimates concentrations with the dispersion equation.

References:

- Ludwig (1983; 1984)
- Ludwig et. al. (1977)

4.2 Model Components and Alternative Formulations

Section 2.0 included discussion of some of the differences in models that would be required to simulate air toxics releases. In Section 3.0, a decision tree (Table 3-2) was presented which defines certain modules which should be included in models given various types of chemical releases. Information on complete models in Table 4-1 can be reviewed to determine if the models can be used to evaluate air toxics emission releases. If the models are inappropriate, the missing or inconsistent component can be modified to provide the appropriate model with a minimum of modifications. The following subsections describe some areas of potential changes.

4.2.1 Source/Emissions Modules

Air toxics releases generally fall into long-term continuous or short-term categories. Often continuous releases can be simulated using generally accepted dispersion models with point or area source terms. Emission rates are determined from field measurements, parameterizations or theoretical models. Short-term releases more often occur as a result of accidental releases or batch type processes for which source estimates are poorly defined and difficult to determine.

Selection of emission parameters for soil related dusts which may have a toxic component can be guided by emission factor relationships developed for the EPA(1984). Equations have been developed for paved and unpaved roads due to wind and vehicular traffic, agricultural tilling, and aggregate handling and storage. Equations consider wind erosion, material types, mechanical action, and soil moisture to determine an emission rate for different conditions. Cox et. al. (1977) discuss an alternative theoretical model for dust emission rate.

Other continuous types of emissions are those due to stack emissions and the volatilization of contaminants on the ground or from storage lagoons. The latter will be discussed with information on short-term releases.

Short-term releases are considered to be of five types:

- Emissions from stationary sources

  Short-term releases from stationary sources are defined in terms of emissions and source parameters required for the models in Section 4.1. Emissions data can be determined from measurements or site specific knowledge of the combustion characteristics or process involved. Short-term releases often occur as a result of relief venting as a safety measure. The characteristics of the relief vent or valve can often be obtained from the source in question. Characteristics of the emissions and other source parameters needed for estimates of plume rise may be available as design parameters but the nature of plant upsets as excursions from normal operations suggests the need for a process evaluation following short-term release. Pressure blowdown will be discussed as another category.

- Evaporation of liquids

  Evaporation of liquids has been simulated with a number of models which will be presented later in this section. Evaporation models are typically derived for evaporation from confined pools or confined spills on land. The first element of the estimate is a determination of the liquid release rate. In general standard fluid dynamical equations are used with simplifying assumptions. The Chlorine Institute (1982) uses an expression in which release rate of the liquid is proportional to the area of the release, a discharge coefficient for orifices and nozzles and the square root of the product of the pressure on the fluid, its density and the gravitational acceleration. Such models are generally not unique nor tested. Models described later in this section describe the release rate in greater detail.

  The basic pool evaporation equations simulate mass transfer by considering the vapor pressure of the liquid, the area of the pool, the energy balance and a mass transfer coefficient. The general form of the equations is discussed by Ille and Springer (1978).

  The pool temperature and mass transfer coefficients represent the primary differences among models and incorporate terms such as the energy balance in the pool and the gas characteristics (e.g. diffusivity). Models can be made time dependent for expanding pools. Shaw and Briscoe (1978) review models for spreading liquids on land. Spreading of liquids on water follows density intrusion models developed for oil spills. The Coast Guard HACS models describe source models of this type.

- Vaporization of liquefied gases (cryogenic)

  Cryogenic liquefied gases have been studied due to the interest in LNG. Pool models for land spills and water spills have been developed based on measurements of LNG vaporization and theoretical models for heat conduction. Heat conduction from the ground is considered the most important heat source and models for land spills are solutions of one dimensional heat conduction equations. A common form of equation for vaporization rate per unit area is given by Shaw and Briscoe (1978).

  Other models consider additional heat sources such as the latent heat of fusion and solar insolation. Total emission rates are given by a number of different assumptions including:

  - for unconfined continuous spills, vaporization equals liquid release rate

  - the area of vaporization is equal to the area of confinement.

  - the spill area can be determined from the pool spreading speed.

Spills on water use similar models with density intrusion models to represent liquid spreading and vaporization based on heat transfer which is enhanced by convection in the water. An example model for continuous spills on water is given by (Shaw and Briscoe, 1978).

Most data available are for LNG experiments on both land and water. In many cases, the data and the models are not easily transferable because the data are given in terms of LNG regression rate. Differences between LNG and other chemical vaporization models include primarily a question of what are the most important variables to be considered in energy balances and whether ice (and related latent heating) is formed by spills on water.

- Pressurized liquified gas spills

The accidental, short-term release of pressurized gases is one of the most difficult types of release to simulate. Since the gas is stored under pressure, the boiling point is raised to a level above ambient temperature. On release of the pressure, by damage to the pressure vessel or piping, the pressure is reduced and the boiling point is lowered to the value for ambient atmospheric pressure. With the rapid drop in pressure, a significant portion of the liquid is adiabatically flash vaporized to gas and the temperature of the remaining pool or tank volume is reduced to the boiling point. For chlorine, the amount of gas flashed is 30 to 25 percent of its initial volume depending on the initial storage temperature. The amount can be determined through thermodynamic calculations.

If the tank damage is above the liquid level, gas will escape to the atmosphere and the remaining liquid will evaporate as heat is obtained from its surroundings. This gas release rate is relatively small. If the tank damage is below liquid level or if there is a complete and rapid failure, large portions of this initial volume will be entrained as very small droplets into the vapor from the vigorous boiling. The size of the droplets is small enough to avoid gravitational settling and their evaporation in the cloud-entrained air reduces the cloud temperature to the boiling point. This reduction can be sufficient to make the cloud negatively buoyant with respect to air. Complex two-phase flow models are available for releases from pipes. In the case of catastrophic tank failures little is known about the entrainment of droplets and it is sometimes assumed that the entire tank contents are flashed or entrained into the initial cloud. Kansa et al. (1983) report an attempt to simulate the transitional density of an ammonia vapor/droplet cloud given an initial estimate of the liquid fraction.

- Pipeline ruptures

Models have been developed to estimate the source rate of gas released from a pipeline leak or failure (Hanna and Munger, 1983; Blewitt, 1985). The models consider the characteristics of the gas and opening and the mass available between the failure and block valves to provide a time dependent emission rate.

Vapor discharge rates can be calculated by standard equations. For example, the Chlorine Institute (1982) presented an equation for vapor discharge.

Table 4-2 identifies and lists the characteristics of source models identified in this study. The majority of available source models are for pool evaporation of specific chemicals such as propellants. A major source for models of vaporization for a large range of source conditions is the U.S. Coast Guard HACS system.

4.2.2 Chemical Conversions

Chemical modules have traditionally been included in air quality models to simulate photochemistry related hydrocarbon, NO_x and oxidant emissions. Losses of material have also been included in models by a simple exponential decay parameter based on a constant conversion rate. Few models discussed here have chemical conversion/reaction modules, although an understanding of chemical and combustion products may be very important in air toxics impact assessments.

4.2.3 Deposition

Deposition from plumes may be important both because of the potential impact of the materials deposited and the loss of material from the plume. Dry deposition is controlled by the transfer characteristics of the atmosphere, the chemical and physical characteristics of the depositing material, and the characteristics of the surface. Atmospheric factors govern the rate at which pollutants are transferred through the atmosphere to the surface. The pollutant characteristics determine if the pollutant will act as an aerosol or gas and whether it reacts with the surface to enhance the deposition rate (e.g. if a gas is soluble in water). The surface

TABLE 4-2

SOURCE CHARACTERIZATION

Characteristics	USCG/ Tang	USAF/ Clewell	NYSDEC/ Shen	Alberta/ Whittaker	Toronto/ Stiver	USAF/ Kahler	ARMY/ Whitacre	USAF/ Ille	Monsanto Wu	Reid (LNG)	UKSRD Shaw
Release											
land	-	X	-	-	X	X	X	X	X	X	X
water	X	-	X	X	-	-	-	-	X	-	X
continuous	-	X	X	X	X	X	X	X	X	X	X
instantaneous	X	-	-	-	-	-	-	-	X	-	X
confined	-	X	X	-	X	X	X	X	X	X	X
unconfined	X	-	-	-	X	-	-	-	X	-	X
pressurized	-	-	-	X	-	-	-	-	-	-	-
cryogenic	-	-	-	-	-	-	-	-	-	X	X
gas	-	-	-	X	-	-	-	-	-	-	-
liquid	X	X	X	-	X	X	X	X	X	X	X
pipeline failure	-	-	-	X	-	-	-	-	-	-	-
tank leak	-	-	-	-	-	-	-	-	X	-	-
tank failure	-	-	-	-	-	-	-	-	X	-	-
Model											
pool evaporation	X	X	X	-	X	X	X	X	X	X	X
steady state	-	X	X	X	X	X	X	X	X	-	-
time dependent	X	-	-	-	X	-	-	-	X	X	X
flashing	-	-	-	-	-	-	-	-	-	-	-
aerosol generation	X	-	-	-	-	-	-	-	-	-	-
plume rise	-	-	-	-	-	-	-	-	-	-	-
empirical	-	-	-	-	-	X	-	-	-	-	-
semiempirical	X	X	-	-	-	-	-	-	-	-	-
analytical/ numerical	-	-	X	X	X	-	X	X	X	X	X
chemical reactions	-	X	-	-							
Inputs/Parameterizations											
area	-	X	X	X	X	X	X	X	X	X	X
wind speed	-	X	X	-	-	X	X	X	X	-	-
stability/ turbulence	-	-	-	-	-	-	X	X	-	-	-
heat exchange:	-	-	-	-	-	-	-	-			
insolation							-	X	X	-	-
substrate							X	X	X	X	X
ice formation							-	-	-	-	-
air: convective						-	X		X	-	-
radiative							-	X	X	-	-
evaporation							-	-	X	-	-
substrate type	-	-	-	-	-	-		X	-	X	X
roughness	-	-	-	-	-	-	X	X	-	-	X
pool temperature	-	X	X	-	X	-	X	X	X	X	X
pressure	-	-	X	X	-	-	-	X	-	-	-
vapor pressure	-	-	-		X	X	X	X	X	-	X

characteristics help determine the meteorological parameters as well as determining the mode of deposition.

Dry deposition parameters or velocities are typically determined by experimentation. Deposition velocity is a parameter made up of a ratio of deposition flux to the surface to the ambient pollutant concentration. In the simplest case, a flux can be determined by multiplying an ambient concentration times a deposition velocity. Deposition velocities, particularly for exotic chemicals, are poorly defined. McMahon and Denison (1979) and Sehmel (1980) have reviewed available data.

The simplest approach to deposition estimates is an exponental decay model:

$$C = C_o \, e^{-\left[\frac{v_d \, t}{\Delta Z}\right]}$$

where v_d is the deposition velocity, t is time and ΔZ is a characteristic depth often given as

$$\Delta Z = \frac{\pi}{2} \sigma_z$$

Wet deposition parameterizations can also use the simple exponential decay parameterization with either of two parameters, a scavenging coefficient, which is simply a fractional scavenging rate, or a washout ratio (W) (the ratio of pollutant concentration in precipitation to that in air). For scavenging coefficients(Λ):

$$C = C_o \quad e \quad (-\Lambda t)$$

where C is the resultant concentration after the scavenging of initial concentration, C_o. This concentration can be calculated using a standard

model without scavenging. For washout ratio W, a scavenging coefficient can be formed by

$$\Lambda \propto \frac{WP}{H}$$

where P is the precipitation rate, H, the depth over which scavenging occurs. The proportionality can be removed by using density corrections to provide Λ in the proper units.

Scavenging coefficients and washout ratios for many materials are reported by McMahon and Denison (1979). Dana et al (1984) describe a program of measurements specifically designed to evaluate scavenging parameters for a limited number of air toxic pollutants based on solubilities.

4.2.4 Plume Rise

Buoyant and momentum plume rise equations are included in most of the EPA preferred models. These equations developed by Briggs are appropriate to most types of air toxic pollutant releases. A summary by Briggs (Randerson, 1984) provides guidance for plume rise estimates for special cases such as plume rise from multiple sources, stack tip downwash, and rise of moist plumes (latent heating effects).

4.2.5 Peak Concentration Levels

Most models for air toxics impact assessments are simplified analytical solutions to advection/diffusion equations representing mean concentrations over some averaging time. Briggs (1973) reports power laws that relate maximum concentration relative to 30-min values and averaging times with exponents ranging from -2/3 to -1/6 depending on atmospheric stability. Some

American Gas Association tests (1967, 1974) indicate peak-to-mean ratios of about 2 or 3.

Care must be exercised in interpreting peak-to-mean ratios. Determinations should be made as to whether the peak values are being ratioed to the maximum value along the centerline of the plume or to an average value off the centerline of the plume. Ramsdell and Hinds (1971) studied a plume from a continuous source and reported fluctuations based on 38-sec time intervals. They observed peak-to-mean ratios greater than 5 less than 1/2% of the time at the plume centerline, whereas ratios of 5 or greater occurred more than 6% of the time near the edge of the mean plume. Terrain effects and atmospheric stability can strongly influence these ratios.

4.2.6 Downwash

Aerodynamic downwash of plumes can be very significant in increasing near-source pollutant concentrations. A limited model adjustment for building downwash is found in ISC, an EPA model described in the previous section. Downwash effects include reduction of plume height, potential recirculation of pollutants in wake cavities, and enhanced initial mixing. The scope of the effects varies significantly with the nature of the obstruction. Hosker (Draxler, 1984) provides a good summary of flow disturbances and the modeling assumptions used in cases with simple geometry.

5.0 MODEL EVALUATIONS

Models for air toxics impact assessments have not been widely evaluated for specific applications. Modeling can involve simulations of phenomena for which appropriate experimental data bases are not available. Most air toxics simulations depend on standard dispersion models either recommended for use by the EPA or which have received implied scientific approval by their continued use over long periods. These models are primarily those developed for the simulation of neutral buoyancy pollutant releases. The predictability of these models is discussed in Section 5.1. Models for the dispersion of pollutants with transitional or negative buoyancy have received less scrutiny due to the dearth of evaluation experiments and the specificity of their applications and testing. Evaluation of these models is discussed in Section 5.2.

5.1 Model Limitations and Uncertainties - Models for Neutrally Buoyant Emissions

Dispersion models contain many simplifications and generalizations, relative to actual plume behavior for a given source at a given time. The pollutant concentrations predicted by a model should be regarded as estimates, subject to error and uncertainty. It is a fairly simple task to enumerate factors which limit a model's accuracy, but it is much more difficult to quantify model uncertainty. Results from a number of model evaluation studies, however, provide a means of characterizing model reliability and of identifying critical areas for future model improvement.

Issues relating to model performance of particular concern for air toxics impact assessments include the estimating of peak (short-term) concentrations,

the spatial distribution of concentration patterns, estimating concentration frequency distributions (mean, median, and extreme values), applications involving complex terrain, performance for very unstable (Class A) dispersion conditions, and performance for negatively buoyant emissions.

5.1.1 Factors Limiting Model Accuracy

The assumptions and simplifications built into a model impose basic limitations on prediction accuracy. A number of these model assumptions are not strictly satisfied in many model applications. Beychok (1979) provides a relatively clear and thorough discussion of the Gaussian model and the conditions for which it is appropriate. Assumptions which are often important limitations include the following:

- Meteorological conditions are assumed to be constant during a given hour. The effects of any systematic change or trend in wind speed, wind direction, or stability conditions during an hour are not described by the model.
- Winds and turbulence are assumed to be the same at all locations throughout the boundary layer. The effects of wind speed or wind direction shear, or of changes in turbulence with height, are not considered within the Gaussian formulation.
- The basic model averaging time is assumed to be long, in comparison to the time scale of turbulent atmospheric motion and in comparison to the transport time from source to receptor.
- Source emissions characteristics are assumed constant over the 1 hour averaging time.
- Pollutant mass is conserved within the Gaussian formulation. Processes which add or remove mass, such as deposition, decay, or chemical transformations, are assumed to be of secondary importance.

A number of models (built on the Gaussian framework) contain provisions for treating conditions which are not consistent with the assumptions noted above. "Retrofit" treatment of the effects of wind shear, gravitational settling and deposition, for example, should be recognized as greatly

simplified approaches to describing these complex phenomena. Numerical models avoid many of these shortcomings and incorporate fewer assumptions. These models, however, are resource and data intensive.

Complex terrain applications pose special difficulties for simple models. Assumptions of straight-line flow ignore the effect of terrain obstacles and can lead to incorrect predictions of plume location and unrealistic concentration estimates, particularly for peak short-term values.

For very unstable conditions, the spatial and temporal scale of atmospheric turbulence increases and assumptions of homogeneous turbulence or long averaging times are generally not satisfied. These conditions also present a formidable challenge to modelers.

Meteorological Factors. For many locations, meteorological conditions are generally consistent with Gaussian model assumptions. For some conditions, however, model predictions should be considered suspect. At very low wind speeds, for example, several model assumptions break down. Pronounced wind direction meander, on a 10- to 30-minute time scale, produces similar problems, as does large wind direction shear (particularly for elevated sources).

Geographical Factors. The Gaussian formulation is consistent with homogeneous terrain/surface roughness and surface radiative properties. Regions where terrain and/or surface conditions are highly variable or undergo an abrupt transition pose considerable difficulties. Examples of problem areas include coastal regions, mountainous regions, rural/urban transition areas, and even forested versus cleared regions. Different sets of dispersion coefficients have been developed for urban and rural regions; how conditions in a given region compare to those for which the coefficients were developed will also influence model reliability.

5.1.2 Operational Uncertainty

Considering the number of factors which contribute to model uncertainty, the prospects of assessing reliability by calculating their combined effects are quite discouraging. A more practical method of assessing model reliability is to compare model predictions with observed air quality. A number of model evaluation studies have involved systematic comparisons of predicted and observed concentration values for a variety of source types and meteorological conditions. Draxler (Randerson, 1985) provides a description of data bases which can be used in evaluations of neutral buoyancy dispersion models.

Such operational tests of model performance are, of course, subject to the limitations of measurement uncertainty and experimental design. Differences between model predictions and observations may be due to uncertainties in model inputs or measured concentrations, in addition to model deficiencies. For most model evaluation studies, care is taken to obtain the best available data sets in order to minimize these effects.

Differences may also result from the natural "noise level" produced by the random fluctuations which characterize atmospheric turbulence. The Gaussian model predicts "expected values" based on a postulated probability distribution of concentrations, but the measured value for a given event represents only a single sample from this distribution. Such "inherent model uncertainty" will set a lower limit to the discrepancies between observed and predicted values.

Operational model evaluation studies have been conducted using data bases ranging from atmospheric tracer dispersion experiments to long-term air quality monitoring programs for actual pollutant sources. Tracer experiments offer the benefits of idealized, well-controlled conditions, while studies for actual sources test the models under "real-world" conditions.

Londergan, et al. (1980) assembled an archive of historical tracer experiments representing a wide range of dispersion conditions and evaluated available regulatory models for urban and rural applications. Most of the data sets represented either near-ground or elevated, fixed-height releases. In a second study, Schulman and Scire (1982) evaluated the EPA models RAM and ISC using a data set of SO_2 measurements taken around an industrial source complex at Midland, Michigan. Comparisons of observed and predicted concentrations for a specific time and location showed large scatter and low correlation. Schulman and Scire found that comparisons of peak concentration values, regardless of time or location, showed better agreement between predictions and observations. The meteorological conditions associated with peak predictions often did not match those for peak observed values.

The Electric Power Research Institute's Plume Model Validation and Development project (Bowne, et.al. 1983) represents an extensive program of field experiments and evaluation studies for tall-stack buoyant plumes. Tracer releases from actual power plants were combined with air quality measurements on the ground and aloft to document plume behavior and resulting concentrations for two coal-fired power plants. The first site, the Kincaid plant in central Illinois, is a flat, rural location. Over 300 hours of tracer measurements were made and over 8 months of SO_2 measurements were acquired with a 28-station network of monitors.

Figure 5-1 illustrates the comparison of maximum hourly tracer concentrations predicted by the CRSTER model (an EPA Guideline model) with values measured by the 200-sampler tracer array. The scatter between predicted and observed concentrations is readily apparent. The observed and predicted cumulative distributions of tracer concentrations are illustrated in Figure 5-2. While systematic differences are evident, differences between the

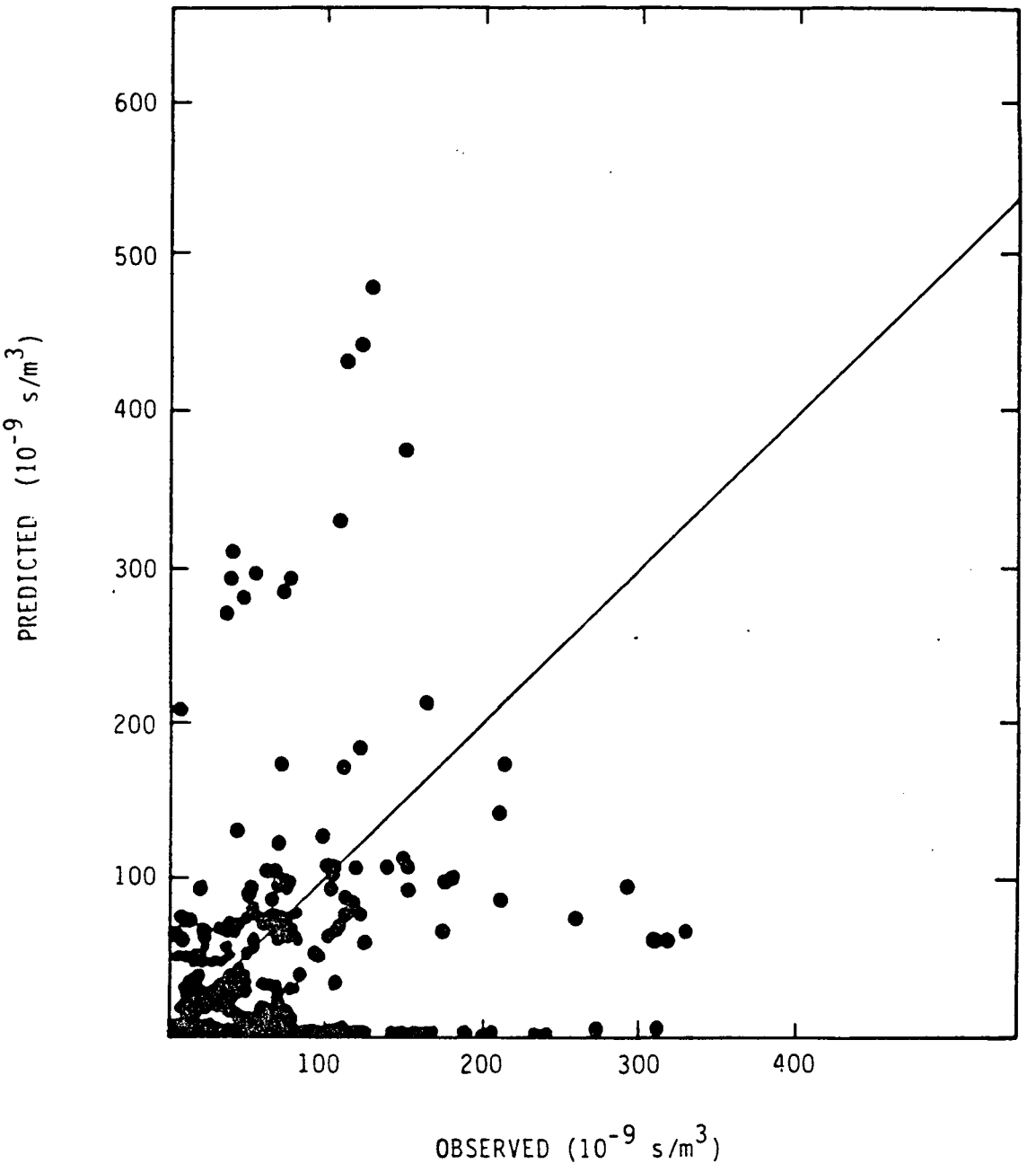

Figure 5-1. Comparison of highest observed and predicted relative concentrations (χ/Q; concentration/emission rates) values for paired one-hour concentration averages from the CRSTER continuous Gaussian Point Source Model showing the typical scatter in paired comparisons.

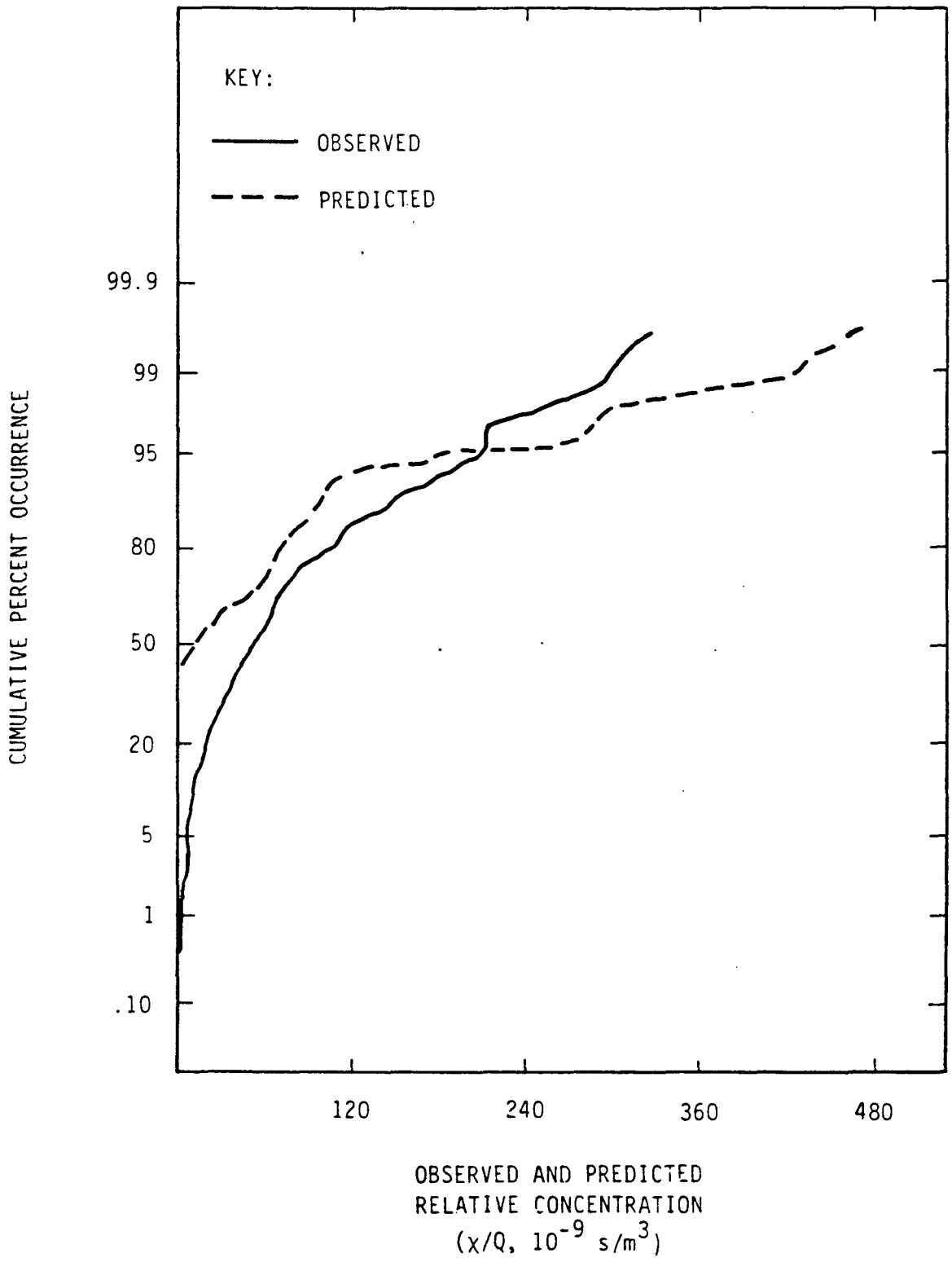

Figure 5-2. Cumulative frequency distributions of the highest observed and predicted χ/Q values for one-hour average concentrations using the CRSTER model. The plots show more agreement in frequency distributions than was found in one-to-one pairings in the previous figure.

distributions are generally smaller than those indicated for event-by-event comparisons.

EPA has sponsored a series of systematic model performance evaluation studies for regulatory models. An AMS workshop on model validation (Fox, 1980) recommended a statistical approach for validation studies. A group of seven rural models (Londergan, et al., 1982) were evaluated following this approach, using data from a six-station SO_2 network around the Clifty Creek power plant in Indiana. Six urban models (Minott, et.al., 1983) were then evaluated using one year of SO_2 data (13 stations) from the St. Louis RAPS study. A group of eight complex terrain models were evaluated (Wackter and Londergan, 1984) using two data sets, including tracer experiments conducted at Cinder Cone Butte, an isolated hill in Idaho, plus measurements taken around the Westvaco Luke paper mill in western Maryland.

All of these studies have indicated similar limitations for models in present use. Comparisons between observed and predicted concentrations paired in time show large scatter and low correlation (generally 0.2 or less). Measurements for actual sources show more scatter than those for idealized tracer experiments. The meteorological conditions associated with peak observed and predicted values often do not match. For rural and urban applications, peak predicted concentrations (regardless of time) generally matched observed peak values within a factor of 2. For complex terrain, however, the Complex I model (currently recommended by EPA as a screening technique) over-predicted peak concentrations for Westvaco by a factor of 10.

For long-term average concentrations, model performance varies with source and terrain characteristics. For distributed low-level sources in uncomplicated terrain, model predictions often agree with observed concentrations within 20 to 30 percent. This level of performance has been achieved in urban studies, such as Minott, et al (1983). For elevated

point-source emissions, regulatory models have been found to underpredict long-term average values substantially. This problem is particularly evident in complex terrain settings.

5.1.3 Reliability of Model Components

An understanding of the reliability of individual model components and of the sensitivity of model predictions to these components is an essential first step in efforts to improve current models. Several studies aimed at developing improved models have examined components such as plume rise and horizontal and vertical dispersion coefficients.

The EPRI Plume Model Validation and Development project undertook a systematic "diagnostic model validation" (Liu, et al., 1982) of the basic components of models applied to tall-stack plumes, including a model sensitivity analysis which identified plume rise and vertical dispersion coefficients as the variables which influence predicted ground-level concentration most strongly (and contribute most to model uncertainty). Based on remote-sensing (lidar) measurements of plume height and dimensions aloft at the Kincaid site, both the plume rise and σ_z algorithms were found to contain systematic biases, with predictions differing from observed values by an average of 20 to 40 percent.

In a follow-up study using the historical tracer data archive, Londergan et al., (1982) compared predicted and observed dispersion coefficients for near-ground release tracer experiments. One important finding from these comparisons is the critical role which stability classification plays in the prediction of dispersion coefficients. For horizontal dispersion, prediction schemes using measured horizontal turbulence to estimate σ_y were more reliable than the standard Turner method based on wind speed and solar radiation.

When the uncertainties in individual model components are examined separately, it is sometimes surprising that Gaussian models perform as well they do. The interdependence of different components, through formulas which depend upon the same model inputs (such as stability class), often leads to compensating errors which reduce the effect on predicted concentrations. For example, the EPRI Kincaid study found that both plume rise and vertical dispersion were generally over-predicted, and the effects of these errors (on ground-level concentrations) were partially offsetting.

5.2 Model Limitations and Uncertainties - Air Toxics Models

Much of the previous discussion focused on difficulties and uncertainties associated with models for relatively well behaved gases or, at least, well controlled sources. These models assume that steady-state release and dispersive conditions exist and that the dispersing material behaves like a neutral buoyancy tracer. From these models, mean concentrations are calculated. Point-by-point comparisons of observations and predictions indicate that model performance is limited. Modeling for most air toxics applications uses the same capabilities and assumptions identified for air quality models and is therefore subject to the same level of uncertainties. Other modeling applications require consideration of a list of additional model assumptions and constraints to cover such phenomena as:

- heavy gas dispersion
- time varying release rates
- effects of warming cold gas clouds
- liquid evaporation and liquified gas vaporization

Each constraint adds a different set of requirements to modeling and the potential for increased uncertainties.

Model evaluation for dense gas releases has been attempted. The evaluations are often chemical specific and suffer from inadequate data bases. These problems occur because generation and dispersion of many dense/toxic gases is scale dependent which requires testing of actual chemicals at full or at least large scale. Often the number of tests is so limited that variations of even the main model parameters cannot be thoroughly examined through final test results.

The references listed in Reference Sections R.2 and R.3 provide a description of some experimental programs and previous model evaluations. Results for the most part are limited to tests and models for heavy gas dispersion, particularly LNG. Experiments with LNG were difficult to control, particularly at the source. In many cases, they were of a scale too small to demonstrate gravity spreading. In some larger experiments, gravity spreading was identified but gravity effects dominated atmospheric turbulence effects only on limited occasions. Models were compared to these data with the result that the simple models conservatively overpredicted the distance of the maximum impact zones. The modules were not designed nor were they effective in simulating high frequency fluctations in pollutant concentrations.

6.0 SUMMARY

This report deals with air toxics impact assessments. The primary assessment tools considered are models to simulate releases of air toxics and subsequent dispersion. The scope of the report is very broad in that impact assessments may be needed for a large variety of pollutants over time periods from a few minutes to many years. To provide a more manageable perspective, the report is bounded by considering only dispersion models of the scale which could reasonably be expected to provide clear impact assessments in the event of air toxics pollutant emissions from a single source. This is not meant to imply that the models always provide unambiguous assessments, but rather that the models as a class represent dispersion over scales typically representative of air toxics impacts. The resulting collection of models is most generally representative of dispersion over distances up to fifty kilometers from the release point.

Model descriptions are prepared by combining information on EPA models, developed for regulatory applications, with models for unique applications developed for chemical modeling. In general, EPA models are identified in this report where the model assumptions are appropriate for air toxics assessments. The literature review provides descriptions of additional models in the following categories:

- source models for estimating emissions for toxic and flammable materials spills (particularly pool evaporation models)
- dispersion models tied to multimedia models for impact assessments.
- models not limited by standard assumptions of typical Gaussian models (e.g. models for instantaneous sources, models for depositing chemicals)
- models for the disperson of chemicals which are negatively buoyant with respect to air or those with transitional buoyancy.

A general conclusion from the literature survey is that no single, available model can completely simulate all air toxics impacts. The variety of chemicals and release scenarios requires a variety of models. Development of non-traditional dispersion models has been sporadic in response to needs related to individual chemicals or industries. For example, models for heavy gases were oriented initially toward liquefied gaseous fuels and were developed at a time of oil shortage.

A second and related result of the literature survey is that the models currently identified for air toxics impact assessments are inadequately evaluated. Studies assessing air quality models have been progressing with mixed results, but very little data for non-traditional model evaluations is generally available. This finding is related to the specificity of experiments to individual chemicals (most notably LNG). Also, there are difficulties in conducting experiments for pollutants that may be toxic, flammable, depositing, and/or chemically reactive. Findings from available studies have indicated that for many chemicals, dispersion behavior is scale dependent and pollutant specific. These findings indicate that experimental programs must be of large size and must be performed with the chemicals of interest. The costs and logistical problems associated with such large-scale programs have often been prohibitive.

REFERENCES

The following references are provided to support information presented in the report and to provide additional information on available models. The reference list is divided into three sections to identify information on modeling, field experiments used to evaluate models, and model evaluations. The latter section is beneficial since evaluation of models identified herein is beyond the scope of the report.

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16. ABSTRACT

This report identifies models that are available for toxics impact assessments and factors that should be considered in selecting models for specific applications. There is no claim as to the merits of individual models or that the list of models is comprehensive. This report only provides information that may be considered useful to air pollution control programs concerned with air toxics and should not be construed as providing regulatory guidance.

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